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* * * * * * * * * * * Welcome to STN International
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NEWS
      2 DEC 01
                 ChemPort single article sales feature unavailable
NEWS 3 APR 03 CAS coverage of exemplified prophetic substances
                 enhanced
NEWS
     4 APR 07
                 STN is raising the limits on saved answers
NEWS 5
         APR 24
                 CA/CAplus now has more comprehensive patent assignee
                 information
NEWS 6 APR 26 USPATFULL and USPAT2 enhanced with patent
                 assignment/reassignment information
NEWS 7 APR 28 CAS patent authority coverage expanded
NEWS 8 APR 28 ENCOMPLIT/ENCOMPLIT2 search fields enhanced
NEWS 9 APR 28 Limits doubled for structure searching in CAS
                 REGISTRY
NEWS 10 MAY 08 STN Express, Version 8.4, now available
NEWS 11 MAY 11 STN on the Web enhanced
NEWS 12 MAY 11 BEILSTEIN substance information now available on
                 STN Easy
NEWS 13
         MAY 14 DGENE, PCTGEN and USGENE enhanced with increased
                 limits for exact sequence match searches and
                 introduction of free HIT display format
NEWS 14
         MAY 15 INPADOCDB and INPAFAMDB enhanced with Chinese legal
                 status data
NEWS 15 MAY 28 CAS databases on STN enhanced with NANO super role in
                 records back to 1992
         JUN 01 CAS REGISTRY Source of Registration (SR) searching
NEWS 16
                 enhanced on STN
NEWS 17 JUN 26 NUTRACEUT and PHARMAML no longer updated
NEWS 18 JUN 29 IMSCOPROFILE now reloaded monthly
NEWS 19
         JUN 29
                 EPFULL adds Simultaneous Left and Right Truncation
                 (SLART) to AB, MCLM, and TI fields
         JUL 09 PATDPAFULL adds Simultaneous Left and Right
NEWS 20
                 Truncation (SLART) to AB, CLM, MCLM, and TI fields
NEWS 21
         JUL 14 USGENE enhances coverage of patent sequence location
                 (PSL) data
NEWS 22
         JUL 14 CA/CAplus to be enhanced with new citing references
                 features
NEWS 23
         JUL 16
                 GBFULL adds patent backfile data to 1855
         JUL 21 USGENE adds bibliographic and sequence information
NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
             AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.
```

Page 1

NEWS HOURS STN Operating Hours Plus Help Desk Availability NEWS LOGIN Welcome Banner and News Items

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FILE 'HOME' ENTERED AT 12:22:34 ON 21 JUL 2009

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=> FILE REGISTRY

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.22 0.22

FULL ESTIMATED COST

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STRUCTURE FILE UPDATES: 19 JUL 2009 HIGHEST RN 1165441-73-5 DICTIONARY FILE UPDATES: 19 JUL 2009 HIGHEST RN 1165441-73-5

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

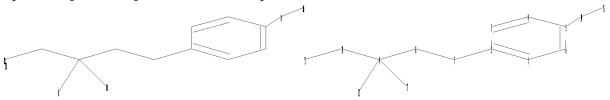
Please note that search-term pricing does apply when conducting ${\tt SmartSELECT}$ searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\Stnexp\Queries\10591774.str



chain nodes :
7 8 9 10 11 12 13 14 16

ring nodes:
1 2 3 4 5 6
chain bonds:

2-7 5-14 7-8 8-9 9-10 9-12 9-13 10-11 14-16

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds : 5-14 9-12 9-13 14-16

exact bonds : 2-7 7-8 8-9 9-10 10-11

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isolated ring systems :

containing 1 :

Match level :

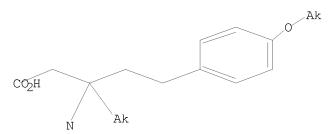
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 16:CLASS

L1 STRUCTURE UPLOADED

=> D L1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

Page 3

10591774.trn 07/21/2009

=> S L1

SAMPLE SEARCH INITIATED 12:23:11 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 119 TO ITERATE

100.0% PROCESSED 119 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 1726 TO 3034

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> S L1 SSS FULL

FULL SEARCH INITIATED 12:23:19 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2403 TO ITERATE

100.0% PROCESSED 2403 ITERATIONS 1 ANSWERS

SEARCH TIME: 00.00.01

L3 1 SEA SSS FUL L1

=> FIL HCAPLUS

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 185.88 186.10

FILE 'HCAPLUS' ENTERED AT 12:23:25 ON 21 JUL 2009
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FILE COVERS 1907 - 21 Jul 2009 VOL 151 ISS 4
FILE LAST UPDATED: 20 Jul 2009 (20090720/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2009.

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10591774.trn 07/21/2009 Page 4

This file contains CAS Registry Numbers for easy and accurate substance identification.

The ALL, BIB, MAX, and STD display formats in the CA/CAplus family of databases will soon be updated to include new citing references information. This enhancement may impact record import into database management software. For additional information, refer to NEWS 22.

=> S L3

1 L3 L4

=> d l4 ibib abs hitstr tot

ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1004693 HCAPLUS

DOCUMENT NUMBER: 143:267240

TITLE: Preparation of amino acid derivatives and

pharmaceutical compositions containing them

Hinterding, Klaus; Hoegenauer, Klemens INVENTOR(S):

Novartis A.-G., Switz.; Novartis Pharma G.m.b.H. PATENT ASSIGNEE(S):

SOURCE: PCT Int. Appl., 24 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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WO	2005085179 W: AE, AG, AL, CN, CO, CR, GE, GH, GM, LK, LR, LS, NO, NZ, OM,			AM, CU, HR, LT, PG,	AT, CZ, HU, LU, PH,	, AU, AZ, , DE, DK, , ID, IL, , LV, MA, , PL, PT,		BA, DM, IN, MD, RO,	BB, DZ, IS, MG, RU,	BG, EC, JP, MK, SC,	BR, EE, KE, MN, SD,	BW, EG, KG, MW, SE,	BY, ES, KP, MX, SG,	BZ, CA, FI, GB, KR, KZ, MZ, NA,	CA, GB, KZ, NA, SL,	CH, GD, LC, NI, SM,			
	R₩:	BW, AZ, EE, RO,	GH, BY, ES, SE,	GM, KG, FI, SI,	KE, KZ, FR,	LS, MD, GB, TR,	MW, RU, GR,	MZ, TJ, HU,	NA, TM, IE,	SD, AT, IS,	US, SL, BE, IT, CI,	SZ, BG, LT,	TZ, CH, LU,	UG, CY, MC,	ZM, CZ, NL,	ZW, DE, PL,	AM, DK, PT,	ΖW	
AU	2005	A1 B2	A1 20050915 B2 20081016 A1 20050915																
EP	1725519 R: AT, BE, BG, IS, IT, LI,			CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	0050. HU,				
BR					А			0731 1206							20050308 20050308				
KR KR	2006010284 2007019702 879831 20070135501				A B1			0215 0122		MX 2006-10284 KR 2006-718344 US 2006-591774						20060908			

PRIORITY APPLN. INFO.:

GB 2004-5289

A 20040309

WO 2005-EP2447

W 20050308

OTHER SOURCE(S): CASREACT 143:267240; MARPAT 143:267240

AB The invention relates to new amino acid derivs. R4R5NCR1R3CH2CH2R2 [R1 is alkyl optionally substituted by OH, alkoxy or F, alkenyl, alkynyl; R2 is R6X-substituted Ph (may be further substituted) or 2-naphthyl, 2-R6X-substituted benzoxazol-5-yl or benzodioxol-5-yl, where X is O, CO, S or a bond and R6 is optionally substituted alkyl or oxa- or oxoalkyl; R3 is -A-B-CO2H, where A and B are independently a bond, CO or CDE (D and E are independently H, halo or alkyl); R4, R5 are independently H, alkyl, haloalkyl or acyl (with provisos)], including their production and use, particularly in transplantation. Thus,

(R)-3-amino-5-[4-(heptyloxy)phenyl]-3-methylpentanoic acid, prepared by a multistep sequence starting from N-Boc-protected

(R)-2-amino-4-(4-hydroxyphenyl)-2-methyl-1-butanol, showed binding affinity to individual human sphingosine 1 phosphate (S1P) receptors (EC50 for binding to S1P1 is 11 nM).

IT 863991-32-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of amino acid derivs. and pharmaceutical compns. containing them)

RN 863991-32-6 HCAPLUS

CN Benzenepentanoic acid, β -amino-4-(heptyloxy)- β -methyl-, (β R)- (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> FIL REGISTRY COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION 17.04 203.14 FULL ESTIMATED COST DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -0.82-0.82

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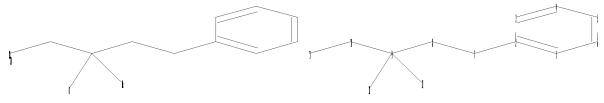
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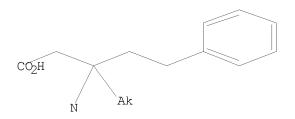
chain nodes : 7 8 9 10 11 12 13 ring nodes : 1 2 3 4 5 6 chain bonds : 2-7 7-8 8-9 9-10 9-12 9-13 10-11 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 exact/norm bonds : 9-12 9-13 exact bonds : 2-7 7-8 8-9 9-10 10-11 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems : containing 1 :

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 15

SAMPLE SEARCH INITIATED 12:26:13 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 302 TO ITERATE

100.0% PROCESSED 302 ITERATIONS 6 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 4998 TO 7082 PROJECTED ANSWERS: 6 TO 266

L6 6 SEA SSS SAM L5

=> s 15 sss full

FULL SEARCH INITIATED 12:26:21 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 6074 TO ITERATE

100.0% PROCESSED 6074 ITERATIONS 68 ANSWERS

SEARCH TIME: 00.00.01

L7 68 SEA SSS FUL L5

=> FIL HCAPLUS

COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
186.36 389.50

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL
ENTRY SESSION

CA SUBSCRIBER PRICE 0.00 -0.82

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FILE COVERS 1907 - 21 Jul 2009 VOL 151 ISS 4
FILE LAST UPDATED: 20 Jul 2009 (20090720/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

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This file contains CAS Registry Numbers for easy and accurate substance identification.

The ALL, BIB, MAX, and STD display formats in the CA/CAplus family of databases will soon be updated to include new citing references information. This enhancement may impact record import into database management software. For additional information, refer to NEWS 22.

=> d his

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FILE 'REGISTRY' ENTERED AT 12:22:56 ON 21 JUL 2009

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 1 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 12:23:25 ON 21 JUL 2009

L4 1 S L3

FILE 'REGISTRY' ENTERED AT 12:25:32 ON 21 JUL 2009

L5 STRUCTURE UPLOADED

L6 6 S L5

L7 68 S L5 SSS FULL

FILE 'HCAPLUS' ENTERED AT 12:26:49 ON 21 JUL 2009

=> s 17

L8 6 L7

=> d 18 ibib abs hitstr tot

L8 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:525259 HCAPLUS

DOCUMENT NUMBER: 148:585420

TITLE: A New Silicon Lewis Acid for Highly Enantioselective

Mannich Reactions of Aliphatic Ketone-Derived

Hydrazones

AUTHOR(S): Notte, Gregory T.; Leighton, James L.

CORPORATE SOURCE: Department of Chemistry, Columbia University, New

York, NY, 10027, USA

SOURCE: Journal of the American Chemical Society (2008),

130(21), 6676-6677

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 148:585420

GΙ

AB The first general method for the highly enantioselective Mannich reaction of aliphatic ketimines is reported. A new, second generation chiral silane Lewis acid has been developed that promotes the reaction between ketone-derived hydrazones and silyl ketene acetals, providing the β,β -disubstituted β -amino esters, e.g., I, with good enantioselectivity even for the hydrazone derived from 2-butanone (Me vs Et, 91% ee). Several examples are provided, including a reaction with a substituted (propanoate-derived) silyl ketene acetal.

IT 1028492-27-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure; stereoselective preparation of (tetrahydroquinolinyl)acetate derivative via chiral silane-catalyzed enantioselective Mannich reaction, reduction, and heterocyclization of (bromophenyl)butanone-derived hydrazone)

RN 1028492-27-4 HCAPLUS

CN Benzenepentanoic acid, 2-bromo- β -methyl- β -[(4-nitrobenzoyl)amino]-, (β S)- (CA INDEX NAME)

Absolute stereochemistry.

PUBLISHER:

34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2009 ACS on STN Γ8

2007:1201261 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 148:54432

TITLE: Asymmetric formation of allylic amines with N-substituted quaternary stereocenters by

PdII-catalyzed aza-Claisen rearrangements

AUTHOR(S): Fischer, Daniel F.; Xin, Zhuo-qun; Peters, Rene

Laboratory of Organic Chemistry, ETH Zuerich, Zurich, CORPORATE SOURCE:

8093, Switz.

SOURCE: Angewandte Chemie, International Edition (2007),

46(40), 7704-7707

CODEN: ACIEF5; ISSN: 1433-7851 Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 148:54432

With $(\mu-C1) 2 [Pd(2-((4R,5R)-4,5-di-tert-butyl-4,5-dihydro-1-tosyl-1H$ imidazol-2-yl)-1',2',3',4',5'-pentaphenylferrocenyl)]2 (containing 1 diastereomer of the ligand) as precatalyst, quaternary N-substituted stereocenters can be generated in an asym. aza-Claisen rearrangement. Excellent enantioselectivities were obtained even if R and R' have a similar or identical size (e.g. 96% ee for CH3/CD3, i.e. conversion of (E)-MeC(CD3):CHCH2OC(CF3):NPMP to (R)-CF3C(O)N(PMP)CMe(CD3)CH:CH2).

ΙT 960060-26-8P, (R)-3-[[[(9H-Fluoren-9-yl)methoxy]carbonyl]amino]-3-

methyl-5-phenylpentanoic acid

RL: SPN (Synthetic preparation); PREP (Preparation)

(asym. formation of allylic amines with N-substituted quaternary stereocenters by PdII-catalyzed aza-Claisen rearrangements)

960060-26-8 HCAPLUS RN

Benzenepentanoic acid, β -[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-CN β -methyl-, (β R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1004693 HCAPLUS

DOCUMENT NUMBER: 143:267240 TITLE: Preparation of amino acid derivatives and pharmaceutical compositions containing them

Hinterding, Klaus; Hoegenauer, Klemens INVENTOR(S):

PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.

SOURCE: PCT Int. Appl., 24 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAI	ENT :	NO.			KIN	D	DATE			APPI	ICAT	ION :	DATE						
WO	2005		A1	_	2005		WO 2005-EP2447						20050308						
											BG,								
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,		
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	KΖ,	LC,		
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,		
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM,		
		SY,	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW	
	RW:										SL,								
		ΑZ,	BY,	KG,	KΖ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,		
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IS,	ΙΤ,	LT,	LU,	MC,	NL,	PL,	PT,		
		RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,		
		MR,	ΝE,	SN,	TD,	ΤG													
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											RO,								
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	2006		-								2006-								
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RITY	APP	LN.	INFO	.:							2004-								
										-	2005-					0050	308		

OTHER SOURCE(S): CASREACT 143:267240; MARPAT 143:267240

The invention relates to new amino acid derivs. R4R5NCR1R3CH2CH2R2 [R1 is alkyl optionally substituted by OH, alkoxy or F, alkenyl, alkynyl; R2 is R6X-substituted Ph (may be further substituted) or 2-naphthyl, 2-R6X-substituted benzoxazol-5-yl or benzodioxol-5-yl, where X is O, CO, S or a bond and R6 is optionally substituted alkyl or oxa- or oxoalkyl; R3 is -A-B-CO2H, where A and B are independently a bond, CO or CDE (D and E are independently H, halo or alkyl); R4, R5 are independently H, alkyl, haloalkyl or acyl (with provisos)], including their production and use, particularly in transplantation. Thus,

- (R)-3-amino-5-[4-(heptyloxy)phenyl]-3-methylpentanoic acid, prepared by amultistep sequence starting from N-Boc-protected
- (R)-2-amino-4-(4-hydroxyphenyl)-2-methyl-1-butanol, showed bindingaffinity to individual human sphingosine 1 phosphate (S1P) receptors (EC50 for binding to S1P1 is 11 nM).
- 863991-32-6P ΙΤ

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of amino acid derivs. and pharmaceutical compns. containing

them)

RN 863991-32-6 HCAPLUS

CN Benzenepentanoic acid, β -amino-4-(heptyloxy)- β -methyl-, (β R)- (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:426562 HCAPLUS

DOCUMENT NUMBER: 142:481829

TITLE: Preparation of amino(phenyl)alkanoic acid derivatives,

addition salts thereof, and sphingosine-1-phosphate

(S1P) receptor modulators

INVENTOR(S): Kohno, Yasushi; Tanioka, Sayoko; Kikuchi, Yoshiaki;

Kinoshita, Miki; Iwanami, Satoru

PATENT ASSIGNEE(S): Kyorin Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 221 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATEN	ON TI	•			KINI)	DATE		i	APPL	ICAT:	DATE					
WO 20	WO 2005044780						A1 20050519				004-	20041108					
W	I: A	E, P	AG,	AL,	ΑM,	ΑT,	ΑU,	ΑZ,	ΒA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
	C	Ν, Ο	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FΙ,	GB,	GD,
	G:	Ε, Θ	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KΖ,	LC,
	L	К, І	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NΙ,
	N	O, N	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
	T	J, 7	ΓM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UΖ,	VC,	VN,	YU,	ZA,	ZM,	ZW
R	RW: B	W, G	GH,	GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
	A	.Z, E	BY,	KG,	KΖ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
	E	Ε, Ε	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IS,	ΙΤ,	LU,	MC,	NL,	PL,	PT,	RO,
	S	Ε, S	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,
	N:	Ε, S	SN,	TD,	TG												
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GΙ

$$R^2$$

$$(CH_2)_m \xrightarrow{R^4} Y - CO_2R^5$$

AΒ Aminocarboxylic acid derivs. represented by the general formula (I) [wherein R1 = each (un) substituted Ph or C1-10 alkyl; R2 = H, halo, trihalomethyl, C1-4 alkyl, C1-4 alkoxy; R3 = H, C1-4 alkyl, Ph; R4 = H, (un) substituted C1-4 alkyl, C2-4 alkenyl, C2-4 alkynyl, C02H, C1-4 alkoxycarbonyl, benzyloxycarbonyl, CH2OCH2CO2H, CH2OCH2CO2R6 (wherein R6 = C1-4 alkyl, benzyl); X = O, S, SO, SO2; m = 2-4; Y = CH:CH, CH2OCH2, (CH2)n (wherein n = an integer of 0-2), CH2OCHCO2R5 (R5 = same as above)], optical isomers, pharmacol. acceptable salts, or hydrates thereof are prepared These compds. are highly effective in controlling a sphingosine-1-phosphoric acid (S1P) receptor. For example, 3-amino-6-[4-(3-benzyloxyphenylsulfanyl)-2-chlorophenyl]-3hydroxymethylhexanoic acid induced the cellular calcium uptake in CHO cells expressing human S1P1 receptor and those expressing human S1P3 receptor with ED50 of <1 μ mol and \geq 10 μ M, resp. The compds. I in vitro induced the activation of extracellular regulatory kinase in CHO cells expressing human S1P receptor and in vivo inhibited the host-vs.-graft rejection in transplant of lymph node in mice. ΙT 852053-21-5P 852055-44-8P,

3-Amino-5-[4-[(4-benzyloxyphenyl)thio]-2-chlorophenyl]-3hydroxymethylpentanoic acid 852055-46-0P, 3-Amino-5-[4-[(4-benzyloxyphenyl)thio]-2-chlorophenyl]-3-(3-benzyloxyphenyl)hydroxypropyl)pentanoic acid 852055-48-2P, 3-Amino-5-[4-[(4-benzyloxyphenyl)thio]-2-chlorophenyl]-3-propylpentanoic acid 852055-50-6P, 3-Allyl-3-amino-5-[4-[(4benzyloxyphenyl)thio]-2-chlorophenyl]pentanoic acid RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(extracellular-regulatory kinase activation inducers; preparation of amino(phenyl)alkanoic acid derivs. as sphingosine-1-phosphate (S1P) receptor modulators)

RN 852053-21-5 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[[3-(phenylmethoxy)phenyl]thio]- (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & \\ & & & & & \\ NH_2 & & & & & \\ HO_2C-CH_2-C-CH_2-CH_2 & & & & \\ & & & & & \\ HO-CH_2 & & & & \\ \end{array}$$

RN 852055-44-8 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[[4(phenylmethoxy)phenyl]thio]- (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{NH}_2 \\ \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ \text{HO}-\text{CH}_2 \end{array}$$

RN 852055-46-0 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro- β -(3-hydroxypropyl)-4-[[4-(phenylmethoxy)phenyl]thio]- (CA INDEX NAME)

RN 852055-48-2 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro-4-[[4-(phenylmethoxy)phenyl]thio]- β -propyl- (CA INDEX NAME)

$$\begin{array}{c} \text{Cl} \\ \text{HO}_2\text{C}-\text{CH}_2 \\ \text{n-Pr}-\text{C}-\text{CH}_2-\text{CH}_2 \\ \text{NH}_2 \end{array} \\ \begin{array}{c} \text{O}-\text{CH}_2-\text{Ph} \\ \end{array}$$

RN 852055-50-6 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro-4-[[4-(phenylmethoxy)phenyl]thio]- β -2-propen-1-yl- (CA INDEX NAME)

Page 15

$$\begin{array}{c} \text{C1} \\ \text{NH}_2 \\ \text{H}_2\text{C} = \text{CH} - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \text{HO}_2\text{C} - \text{CH}_2 \end{array} \\ \begin{array}{c} \text{O-CH}_2 - \text{Ph} \\ \text{O-CH}_2 - \text{Ph} \\ \text{O-CH}_2 - \text{CH}_2 \\ \end{array}$$

IT 852053-22-6P 852053-25-9P 852053-28-2P 852053-35-1P 852053-39-5P 852053-40-8P 852053-41-9P 852053-68-0P 852053-69-1P

852053-89-5P 852053-90-8P 852053-91-9P 852054-08-1P 852054-10-5P 852054-12-7P 852054-14-9P 852054-43-4P 852054-45-6P 852054-46-7P 852054-48-9P 852054-50-3P 852054-52-5P 852054-84-3P 852054-86-5P 852054-88-7P 852054-91-2P 852054-93-4P 852054-95-6P 852054-97-8P 852054-99-0P 852055-01-7P 852055-03-9P 852055-05-1P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of amino(phenyl)alkanoic acid derivs. as sphingosine-1-phosphate (S1P) receptor modulators) RN 852053-22-6 HCAPLUS CN

Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[[3-(phenylmethoxy)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{C1} & \text{O-CH}_2\text{-Ph} \\ & \text{NH}_2 & \\ & \text{HO}_2\text{C-CH}_2\text{-C-CH}_2\text{-CH}_2 \\ & \text{HO-CH}_2 \end{array}$$

● HCl

852053-25-9 HCAPLUS RN

CN Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[3-(trifluoromethyl)phenoxy]- (CA INDEX NAME)

852053-28-2 HCAPLUS RN

Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[[4-CN (phenylmethoxy)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{NH}_2 \\ \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ \text{HO}-\text{CH}_2 \end{array}$$

RN 852053-35-1 HCAPLUS

CN Benzenepentanoic acid, β -amino- β -(hydroxymethyl)-4-octyl-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{NH}_2\\ \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2\\ \text{HO}-\text{CH}_2 \end{array}$$

● HCl

RN 852053-39-5 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro-4-[[3-(phenylmethoxy)phenyl]thio]- β -propyl-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Cl} & \text{O-CH}_2\text{-Ph} \\ \text{HO}_2\text{C-CH}_2 & \text{n-Pr-C-CH}_2\text{-CH}_2 \end{array}$$

● HCl

RN 852053-40-8 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro-4-[[3-(phenylmethoxy)phenyl]thio]- β -2-propen-1-yl-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{Cl} & \text{O-CH}_2\text{-Ph} \\ \text{NH}_2 \\ \text{H}_2\text{C--CH}_2\text{-CH}_2 \\ \text{HO}_2\text{C--CH}_2 \end{array}$$

RN 852053-41-9 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro- β -(3-hydroxypropyl)-4- [[3-(phenylmethoxy)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} & \text{O-CH}_2\text{-Ph} \\ \text{NH}_2 & \text{HO-(CH}_2)_3\text{-C-CH}_2\text{-CH}_2 \\ \text{HO}_2\text{C-CH}_2 & \text{CH}_2 \end{array}$$

● HCl

RN 852053-68-0 HCAPLUS

CN Benzenepentanoic acid, 2-chloro- β -(hydroxymethyl)- β (methylamino)-4-[[3-(phenylmethoxy)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} & \text{O-CH}_2\text{--Ph} \\ \text{NHMe} & \text{HO}_2\text{C--CH}_2\text{--CH}_2\text{--CH}_2 \\ & \text{HO--CH}_2 \end{array}$$

● HCl

RN 852053-69-1 HCAPLUS

CN Benzenepentanoic acid, 2-chloro- β -(hydroxymethyl)- β (phenylamino)-4-[[3-(phenylmethoxy)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} & \text{O-CH}_2\text{-Ph} \\ \text{NHPh} & \text{HO}_2\text{C-CH}_2\text{-CH}_2\text{-CH}_2 \\ \text{HO-CH}_2 & \text{O-CH}_2\text{-CH}_2 \end{array}$$

RN 852053-89-5 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro- β -methyl-4-[[4-(phenylmethoxy)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ \text{NH}_2 \end{array} \\ \text{O-CH}_2-\text{Ph}$$

● HCl

RN 852053-90-8 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro-4-[[4- (phenylmethoxy)phenyl]thio]- β -propyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 852053-91-9 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro- β -(3-hydroxypropyl)-4- [[4-(phenylmethoxy)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

RN 852054-08-1 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[[4-(phenylmethoxy)phenyl]thio]-, (+)- (CA INDEX NAME)

Rotation (+).

RN 852054-10-5 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[[4-(phenylmethoxy)phenyl]thio]-, (-)- (CA INDEX NAME)

Rotation (-).

RN 852054-12-7 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[[3-(phenylmethoxy)phenyl]thio]-, (-)- (CA INDEX NAME)

Rotation (-).

$$CO_2H$$
 $C1$ S O Ph H_2N HO

RN 852054-14-9 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[[3-(phenylmethoxy)phenyl]thio]-, (+)- (CA INDEX NAME)

Rotation (+).

RN 852054-43-4 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[(4hydroxyphenyl)thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{C1} \\ & \text{NH}_2 \\ & \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ & \text{HO}-\text{CH}_2 \end{array}$$
 OH

● HCl

RN 852054-45-6 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[(4methoxyphenyl)thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{NH}_2 \\ \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ \text{HO}-\text{CH}_2 \end{array} \\ \text{OMe} \\ \end{array}$$

RN 852054-46-7 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro-4-[[4-(cyclohexylmethoxy)phenyl]thio]- β -(hydroxymethyl)-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 852054-48-9 HCAPLUS

CN Benzenepentanoic acid, β -amino-4-[(4-butoxyphenyl)thio]-2-chloro- β -(hydroxymethyl)-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{C1} \\ & \text{NH}_2 \\ & \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ & \text{HO}-\text{CH}_2 \end{array}$$

● HCl

RN 852054-50-3 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[(4-phenoxyphenyl)thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{NH}_2 \\ \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ \text{HO}-\text{CH}_2 \end{array} \\ \text{OPh} \\ \end{array}$$

852054-52-5 HCAPLUS RN

CN Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[[4-(phenoxymethyl)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{Cl} \\ \text{NH}_2 \\ \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ \text{HO}-\text{CH}_2 \end{array}$$

● HCl

852054-84-3 HCAPLUS RN

CN Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[(3hydroxyphenyl)thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{C1} & \text{OH} \\ & \text{NH}_2 & \\ & \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ & \text{HO}-\text{CH}_2 \end{array}$$

● HCl

852054-86-5 HCAPLUS RN

Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[(3-CN methoxyphenyl)thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{NH}_2 \\ \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ \\ \text{HO}-\text{CH}_2 \end{array}$$

RN 852054-88-7 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro-4-[[3-(cyclohexylmethoxy)phenyl]thio]- β -(hydroxymethyl)-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 852054-91-2 HCAPLUS

CN Benzenepentanoic acid, β -amino-4-[(3-butoxyphenyl)thio]-2-chloro- β -(hydroxymethyl)-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{C1} & \text{OBu-n} \\ & \text{NH}_2 & \\ & \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ & \text{HO}-\text{CH}_2 \end{array}$$

● HCl

RN 852054-93-4 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[(3-phenoxyphenyl)thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{NH}_2 \\ \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ \text{HO}-\text{CH}_2 \end{array}$$

852054-95-6 HCAPLUS RN

CN Benzenepentanoic acid, β -amino-4-([1,1'-biphenyl]-3-ylthio)-2-chloro- β -(hydroxymethyl)-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Cl} & \text{Ph} \\ & \text{NH}_2 \\ & \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ & \text{HO}-\text{CH}_2 \end{array}$$

● HCl

852054-97-8 HCAPLUS RN

Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[[3-CN (2-phenylethynyl)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{C1} & \text{C} \\ & \text{NH}_2 \\ & \text{HO}_2\text{C} - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ & \text{HO} - \text{CH}_2 \end{array}$$

● HCl

852054-99-0 HCAPLUS RN

Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[[3-CN (2-phenylethenyl)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{C1} & \text{CH-Ph} \\ & \text{NH}_2 & \\ & \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ & \text{HO}-\text{CH}_2 \end{array}$$

RN 852055-01-7 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[[3-(2-phenylethyl)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{C1} & \text{CH}_2\text{-}\text{CH}_2\text{-}\text{Ph} \\ & \text{NH}_2 & \\ & \text{HO}_2\text{C}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_2 \\ & \text{HO}-\text{CH}_2 & \end{array}$$

● HCl

RN 852055-03-9 HCAPLUS

CN Benzenepentanoic acid, β -amino-2-chloro- β -(hydroxymethyl)-4-[[3-(2-oxo-2-phenylacetyl)phenyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & \\ & & & & & \\ NH_2 & & & & & \\ HO_2C-CH_2-C-CH_2-CH_2 & & & & \\ & & & & & \\ HO-CH_2 & & & & \\ \end{array}$$

● HC1

RN 852055-05-1 HCAPLUS

CN Benzenepentanoic acid, 4-[(3-acetylphenyl)thio]- β -amino-2-chloro- β -(hydroxymethyl)-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{C1} & \text{Ac} \\ & \text{NH}_2 \\ & \text{HO}_2\text{C}-\text{CH}_2-\text{C}+\text{CH}_2-\text{CH}_2 \\ & \text{HO}-\text{CH}_2 \end{array}$$

HC1

REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:548899 HCAPLUS

DOCUMENT NUMBER: 141:243786

TITLE: Synthesis of optically active β -alkyl aspartate

via [3,3] sigmatropic rearrangement of

 α -acyloxytrialkylsilane

AUTHOR(S): Sakaguchi, Kazuhiko; Yamamoto, Masahiro; Kawamoto,

Tetsuo; Yamada, Takeshi; Shinada, Tetsuro; Shimamoto,

Keiko; Ohfune, Yasufumi

CORPORATE SOURCE: Graduate School of Science, Department of Material

Science, Osaka City University, Sugimoto, Sumiyoshi,

Osaka, 558-8585, Japan

SOURCE: Tetrahedron Letters (2004), 45(30), 5869-5872

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:243786

AB The synthesis of four types of optically active β -carbon-substituted

analogs of threo- β -hydroxy aspartate (THA) and a

 β -carbon-substituted analog of threo- β -benzyloxy aspartate

(TBOA), which are potent blockers of excitatory amino acid transporters in

the mammalian central nervous system, via the chirality-transferring ester-enolate Claisen rearrangement of α -acyloxytrialkylsilane is

described.

IT 749927-13-7P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);

BIOL (Biological study); PREP (Preparation)

(synthesis of optically active β -alkyl aspartate as glutamate uptake inhibitors in mammalian central nervous system)

RN 749927-13-7 HCAPLUS

CN L-Aspartic acid, 3-methyl-2-(2-phenylethyl)-, (3S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1996:376463 HCAPLUS

DOCUMENT NUMBER: 125:168594

ORIGINAL REFERENCE NO.: 125:31609a,31612a

TITLE: Ethyl N-(diphenylmethylene)glycinate as anionic

glycine equivalent. Monoalkylation, dialkylation and Michael additions under solid-liquid phase-transfer

catalysis

AUTHOR(S): Lopez, Anna; Moreno-Manas, Marcial; Pleixats, Roser;

Roglans, Anna; Ezquerra, Jeus; Pedregal, Concepcion

ΙI

CORPORATE SOURCE: Dep. Chem., Univ. Autonoma Barcelona, Barcelona,

08193, Spain

SOURCE: Tetrahedron (1996), 52(24), 8365-8386

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 125:168594

Ι

GΙ

HO2C O NH

AB Et N-(diphenylmethylene)glycinate undergoes monoalkylations, dialkylations and Michael addns. to ethylenic and acetylenic acceptors under appropriate solid-liquid phase transfer catalysis conditions. Further transformations of the α -disubstituted ketimines leads to α -alkylated aspartic and glutamic acid derivs. HO2CCH2C(NH2)(CO2H)(CH2)nPh and HO2CCH2C(NH2)(CO2H)(CH2)nPh (n = 2, 3), to bicyclic amino acids or derivs. featuring pryazolone and isoxazolone moieties I and II, and to α -substituted (E)-3,4-dehydroglutamic acids. IT 180609-01-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(phase-transfer alkylation, dialkylation, and Michael addition reactions of (diphenylmethylene)glycinate as glycine anion synthon)

RN 180609-01-2 HCAPLUS

CN Aspartic acid, 2-(2-phenylethyl)-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{CO}_2\text{H} \\ | \\ \text{HO}_2\text{C} - \text{CH}_2 - \text{C} - \text{CH}_2 - \text{CH}_2 - \text{Ph} \\ | \\ \text{NH}_2 \end{array}$$

=> FIL REGISTRY COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 56.64 446.14 TOTAL DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE SESSION ENTRY CA SUBSCRIBER PRICE -4.92-5.74

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Property values tagged with IC are from the ${\tt ZIC/VINITI}$ data file provided by ${\tt InfoChem.}$

STRUCTURE FILE UPDATES: 19 JUL 2009 HIGHEST RN 1165441-73-5 DICTIONARY FILE UPDATES: 19 JUL 2009 HIGHEST RN 1165441-73-5

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

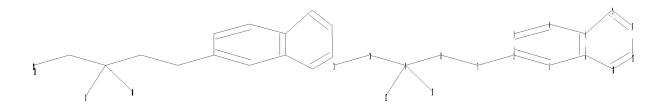
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\Stnexp\Queries\10591774b.str



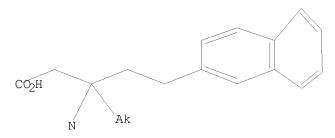
chain nodes : 7 8 9 10 11 12 13 ring nodes : 1 2 3 4 5 6 15 16 17 18 chain bonds : 2-7 7-8 8-9 9-10 9-12 9-13 10-11 ring bonds : $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 5-15 \quad 6-18 \quad 15-16 \quad 16-17 \quad 17-18$ exact/norm bonds : 9-12 9-13 exact bonds : 2-7 7-8 8-9 9-10 10-11 normalized bonds : $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 5-15 \quad 6-18 \quad 15-16 \quad 16-17 \quad 17-18$ isolated ring systems : containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom

L9 STRUCTURE UPLOADED

=> d 19 L9 HAS NO ANSWERS L9 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 19
SAMPLE SEARCH INITIATED 12:31:43 FILE 'REGISTRY'

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10591774

SAMPLE SCREEN SEARCH COMPLETED - 9 TO ITERATE

100.0% PROCESSED 9 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE** BATCH **COMPLETE** 9 TO 360 PROJECTED ITERATIONS:

0 TO PROJECTED ANSWERS: 0

L10 0 SEA SSS SAM L9

=> s 19 sss full

FULL SEARCH INITIATED 12:31:50 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 206 TO ITERATE

100.0% PROCESSED 206 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

L11 0 SEA SSS FUL L9

=> log y

SINCE FILE TOTAL ENTRY SESSION 186.36 632.50 COST IN U.S. DOLLARS FULL ESTIMATED COST

SINCE FILE TOTAL
ENTRY SESSION
0.00 -5.74 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) CA SUBSCRIBER PRICE

STN INTERNATIONAL LOGOFF AT 12:32:25 ON 21 JUL 2009